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Reduced-order model for the BGK equation based on POD and optimal transport

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► **To cite this version:**

Florian Bernard, Angelo Iollo, Sébastien Riffaud. Reduced-order model for the BGK equation based on POD and optimal transport. MOREPAS 2018 - Model Reduction of Parametrized Systems IV, Apr 2018, Nantes, France. hal-02427339

HAL Id: hal-02427339

<https://inria.hal.science/hal-02427339>

Submitted on 3 Jan 2020

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Contribution

We present a model describing a gas flow in both hydrodynamic and rarefied regimes. Since the computational cost of the Bhatnagar-Gross-Krook (BGK) equation can be prohibitive, a reduced-order approximation is developed, leading to fast and accurate simulations.

BGK equation

The dynamics of the gas flow is described by the **BGK equation**:

$$\frac{\partial f}{\partial t}(\mathbf{x}, \xi, t) + \xi \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \xi, t) = \frac{M_f(\mathbf{x}, \xi, t) - f(\mathbf{x}, \xi, t)}{\tau(\mathbf{x}, t)} \quad (1)$$

where f is the density distribution function representing the density of gas particles at point $\mathbf{x} \in \mathbb{R}^3$, velocity $\xi \in \mathbb{R}^3$ and time $t \in \mathbb{R}$. The Maxwellian distribution function M_f is in dimensionless form

$$M_f(\mathbf{x}, \xi, t) = \frac{\rho(\mathbf{x}, t)}{(2\pi T(\mathbf{x}, t))^{\frac{3}{2}}} \exp\left(-\frac{\|\xi - U(\mathbf{x}, t)\|^2}{2T(\mathbf{x}, t)}\right)$$

where $\rho \in \mathbb{R}$ is the density, $U \in \mathbb{R}^3$ is the macroscopic velocity, $T \in \mathbb{R}$ is the temperature and $E \in \mathbb{R}$ is the total energy of the gas.

Reduced-order approximation

The distribution functions are approximated by

$$\tilde{f}(\mathbf{x}, \xi, t) = \sum_{n=1}^{N_{pod}} a_n^f(\mathbf{x}, t) \Phi_n(\xi)$$

and

$$\tilde{M}_f(\mathbf{x}, \xi, t) = \sum_{n=1}^{N_{pod}} a_n^M(\mathbf{x}, t) \Phi_n(\xi)$$

where the basis functions Φ_n are built offline by **Proper Orthogonal Decomposition** (POD) and the coefficients a_n are computed online by the **Galerkin method**.

References

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- [3] F. Bernard, A. Iollo and S. Riffaud. *Reduced-order model for the BGK equation based on POD and optimal transport*. Journal of Computational Physics, 2018.

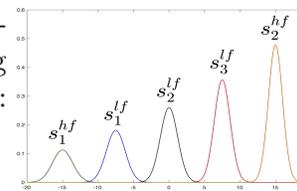
Offline phase

In the offline phase, the BGK equation (1) is sampled to collect information on the distribution functions that we want to approximate. High-fidelity simulations provide snapshots of both the density distribution function and of the Maxwellian distribution function:

$$S^{hf} = \left\{ f(\mathbf{x}_i, \xi, t_k) \right\}_{\substack{1 \leq i \leq N_x \\ 1 \leq k \leq N_t}} \cup \left\{ M_f(\mathbf{x}_i, \xi, t_k) \right\}_{\substack{1 \leq i \leq N_x \\ 1 \leq k \leq N_t}}$$

Then, **optimal transport** provides additional low-fidelity snapshots by interpolating the snapshots of S^{hf} to complete the sampling:

$$S = S^{hf} \cup S^{lf}$$



Finally, the basis functions Φ_n are built by POD to have the best approximation in the least squares sense of the snapshots $s_l \in S$:

$$\begin{cases} \text{minimize} & \sum_{l=1}^{N_{snaps}} \int_{\mathbb{R}^3} (s_l(\xi) - \mathcal{P}[s_l](\xi))^2 d\xi \\ \Phi_1(\xi) \dots \Phi_{N_{pod}}(\xi) & \\ \text{subject to} & \int_{\mathbb{R}^3} \Phi_n(\xi) \Phi_m(\xi) d\xi = \delta_{n,m} \end{cases}$$

where $\mathcal{P}[s_l]$ is the projection of s_l onto the subspace spanned by the basis functions Φ_n (i.e. $\mathcal{P}[s_l](\xi) = \sum_{n=1}^{N_{pod}} \int_{\mathbb{R}^3} s_l(\xi') \Phi_n(\xi') d\xi' \Phi_n(\xi)$).

Online phase

During the online phase, the offline knowledge is used to compute approximations of the distribution functions at low cost. In the Galerkin method, the BGK equation (1) is projected onto the basis functions Φ_n , leading to an **hyperbolic system** of partial differential equations:

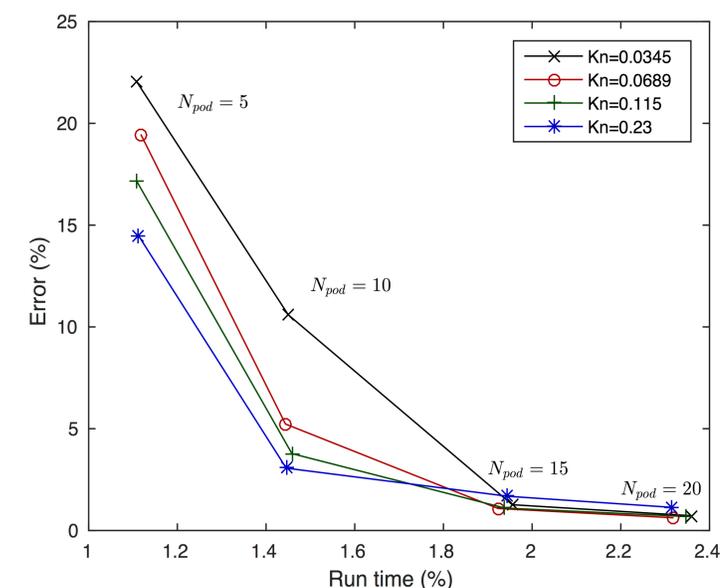
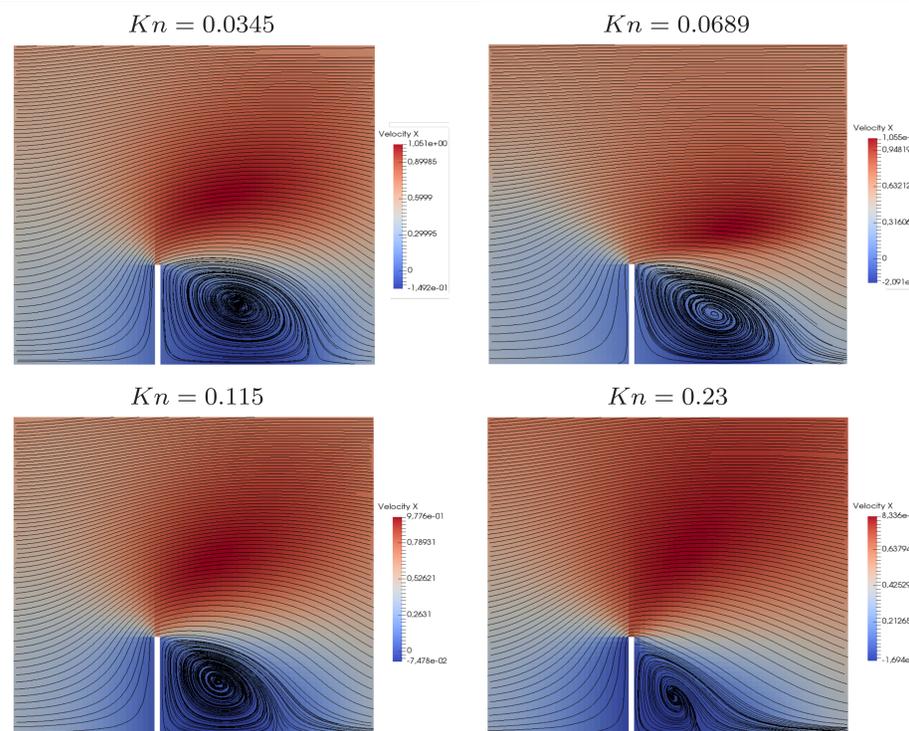
$$\frac{\partial a^f}{\partial t}(\mathbf{x}, t) + A \frac{\partial a^f}{\partial x}(\mathbf{x}, t) + \dot{A} \frac{\partial a^f}{\partial y}(\mathbf{x}, t) + \ddot{A} \frac{\partial a^f}{\partial z}(\mathbf{x}, t) = \frac{a^M(\mathbf{x}, t) - a^f(\mathbf{x}, t)}{\tau(\mathbf{x}, t)}$$

where $a = (a_1, a_2, \dots, a_{N_{pod}})^T$, $A_{n,m} = \int_{\mathbb{R}^3} \xi_u \Phi_n(\xi) \Phi_m(\xi) d\xi$, $\dot{A}_{n,m} = \int_{\mathbb{R}^3} \xi_v \Phi_n(\xi) \Phi_m(\xi) d\xi$ and $\ddot{A}_{n,m} = \int_{\mathbb{R}^3} \xi_w \Phi_n(\xi) \Phi_m(\xi) d\xi$. These equations are decoupled by linear changes of variables and are solved by an **IMEX Runge-Kutta** scheme in time and a **finite volume** scheme in space. To improve the accuracy of the model, the coefficients a_n^M are computed by constrained projection:

$$\begin{cases} \text{minimize} & \int_{\mathbb{R}^3} (M_f(\mathbf{x}, \xi, t) - \tilde{M}_f(\mathbf{x}, \xi, t))^2 d\xi \\ a_1^M(\mathbf{x}, t) \dots a_{N_{pod}}^M(\mathbf{x}, t) & \\ \text{subject to} & \int_{\mathbb{R}^3} \tilde{M}_f(\mathbf{x}, \xi, t) \begin{pmatrix} 1 \\ \xi \\ \frac{\|\xi\|^2}{2} \end{pmatrix} d\xi = \begin{pmatrix} \rho(\mathbf{x}, t) \\ \rho(\mathbf{x}, t)U(\mathbf{x}, t) \\ E(\mathbf{x}, t) \end{pmatrix} \end{cases}$$

in order to **conserve mass, momentum and total energy** of the gas.

Results



In average with $N_{pod} = 20$ basis functions, **the approximation error is less than 1% and the run time is divided by approximately 45** with respect to the high-fidelity simulations.